

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23

ring/chain nodes :

24

chain bonds :

11-18 15-24

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14
13-15 14-17 15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 11-18 12-13
13-14 13-15 14-17 15-16 15-24 16-17 18-19 18-23 19-20 20-21 21-22 22-23

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:CLASS

10/611,785

=> d his

(FILE 'HOME' ENTERED AT 17:19:11 ON 28 JUL 2004)

FILE 'REGISTRY' ENTERED AT 17:19:18 ON 28 JUL 2004

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 0 S L2

L4 83 S L2 SSS FUL

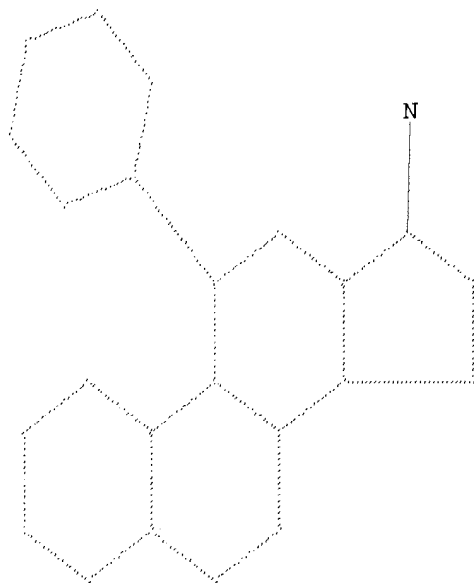
FILE 'CAPLUS' ENTERED AT 17:20:23 ON 28 JUL 2004

L5 3 S L4

=> d 12

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

L2 QUE ABB=ON PLU=ON L1

=> d ibib abs hitstr 1-3

~~15~~ ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:560363 CAPLUS
DOCUMENT NUMBER: 138:147491
TITLE: Identification and characterization of novel estrogen
receptor- β -sparing antiprogestins
AUTHOR(S): Sathya, Ganesan; Jansen, Michelle S.; Nagel, Susan C.;
Cook, C. Edgar; McDonnell, Donald P.
CORPORATE SOURCE: Department of Pharmacology and Cancer Biology, Duke
University Medical Center, Durham, NC, 27710, USA
SOURCE: Endocrinology (2002), 143(8), 3071-3082
CODEN: ENDOAO; ISSN: 0013-7227
PUBLISHER: Endocrine Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The steroid hormones estrogen and progesterone together regulate the development and maintenance of the female reproductive system. The actions of these two hormones are mediated by their resp. nuclear receptors located within overlapping cell populations in target organs. The mol. mechanism of action of these two hormones has been defined to a large extent using estrogen receptor (ER) and progesterone receptor (PR) antagonists. In the case of ER, the available antagonists are highly receptor selective. With respect to PR, however, the available antiprogestins also interact with the receptors for glucocorticoids, mineralocorticoids, and androgens. Whereas these cross-reactivities can usually be managed in studies of female reproductive function, it is the recent demonstration that RU486 is an effective antagonist of the β -isoform of ER that suggested the need for more selective antiprogestins. In this study, we used cell-based transcriptional assays combined with screens using coactivator peptide analogs to identify two novel classes of antiprogestins that distinguish themselves from the antiprogesterin RU486 in the manner they interact with PR. One class exhibits the characteristics of a pure antiprogesterin in that its members bind to the receptor and induce a conformational change that prevents the presentation of two potential coactivator binding surfaces on the protein. The second class of compds. distinguish themselves from RU486 in that they are ER β sparing. When tested in vivo the ER-sparing antiprogestins were as effective as RU486 in suppressing superovulation. It is anticipated that the availability of these new antiprogestins will advance the studies of PR pharmacol. in a manner similar to how the availability of selective ER modulators has helped the study of ER action.

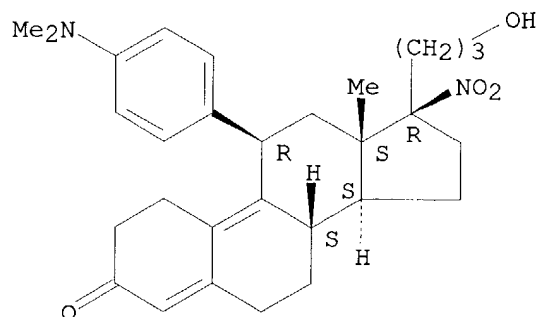
IT 244304-81-2, RTI 6413-015 244304-82-3, RTI 6413-045
244304-85-6, RTI 6413-029E 244304-86-7, RTI 6413-045ox
244304-89-0, RTI 6413-013 244304-91-4, RTI 6413-028
244305-03-1, RTI 6413-044 244305-17-7, RTI 6413-029Z
496840-89-2, RTI 6413-030 496840-92-7, RTI 6413-043
496840-93-8, RTI 6413-043ox

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(identification and characterization of novel estrogen
receptor- β -sparing antiprogestins)

RN 244304-81-2 CAPLUS

CN Estradiol, 11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

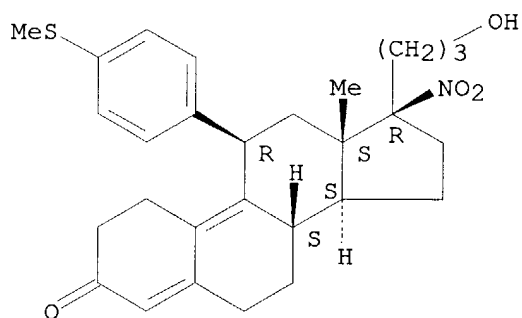
Absolute stereochemistry.



RN 244304-82-3 CAPLUS

CN Estradiol-4,9-dien-3-one, 17-(3-hydroxypropyl)-11-[4-(methylthio)phenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

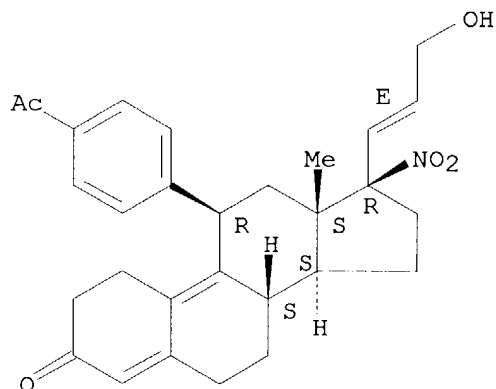


RN 244304-85-6 CAPLUS

CN Estradiol-4,9-dien-3-one, 11-(4-acetylphenyl)-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



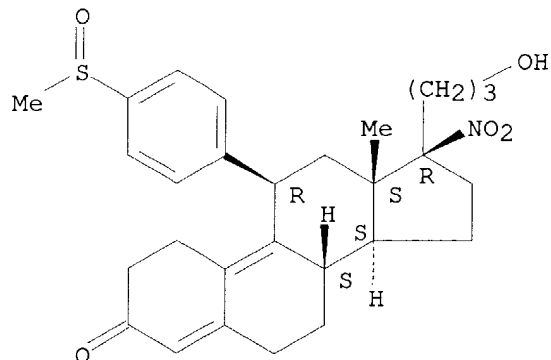
RN 244304-86-7 CAPLUS

CN Estradiol-4,9-dien-3-one, 17-(3-hydroxypropyl)-11-[4-(methylsulfinyl)phenyl]-

10/611,785

17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

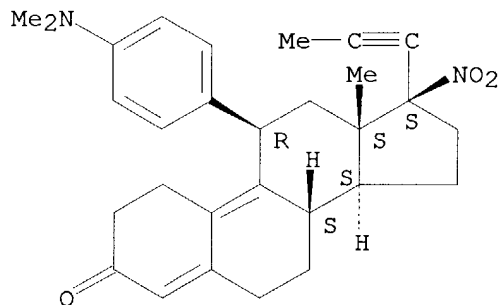
Absolute stereochemistry.



RN 244304-89-0 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-nitro-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

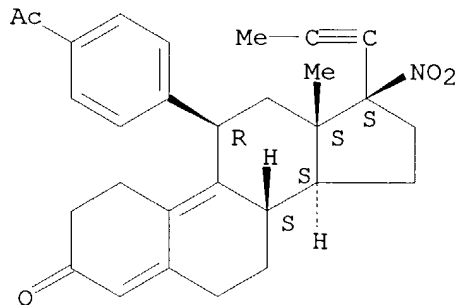
Absolute stereochemistry.



RN 244304-91-4 CAPLUS

CN Estra-4,9-dien-3-one, 11-(4-acetylphenyl)-17-nitro-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



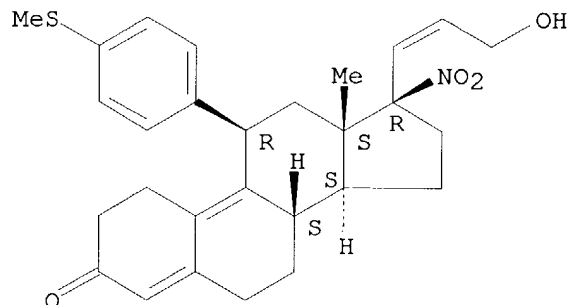
RN 244305-03-1 CAPLUS

10/611,785

CN Estra-4,9-dien-3-one, 17-(3-hydroxy-1-propenyl)-11-[4-(methylthio)phenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

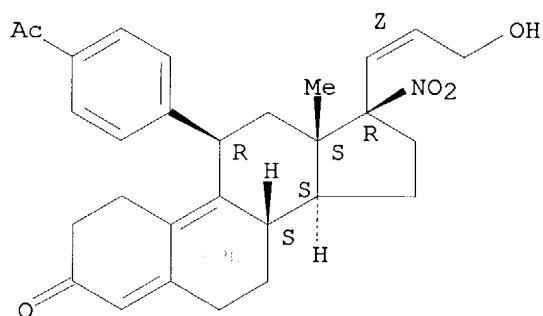


RN 244305-17-7 CAPLUS

CN Estra-4,9-dien-3-one, 11-(4-acetylphenyl)-17-[(1Z)-3-hydroxy-1-propenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

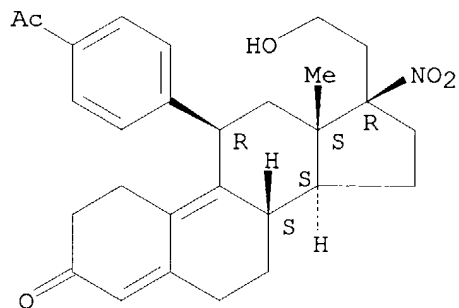
Double bond geometry as shown.



RN 496840-89-2 CAPLUS

CN 19-Norpregna-4,9-dien-3-one, 11-(4-acetylphenyl)-21-hydroxy-17-nitro-, (11 β ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

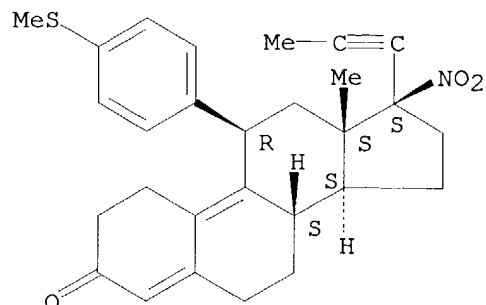


10/611,785

RN 496840-92-7 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(methylthio)phenyl]-17-nitro-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

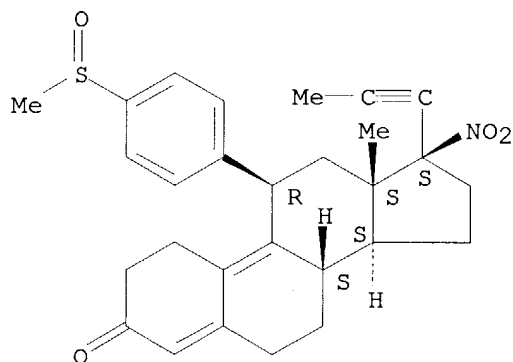


RN 496840-93-8 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(methylsulfinyl)phenyl]-17-nitro-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Currently available stereo shown.



REFERENCE COUNT:

54

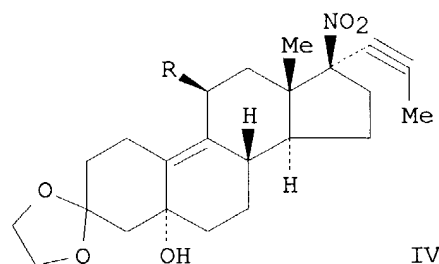
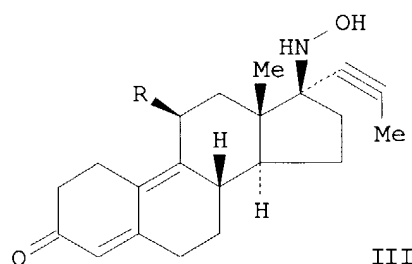
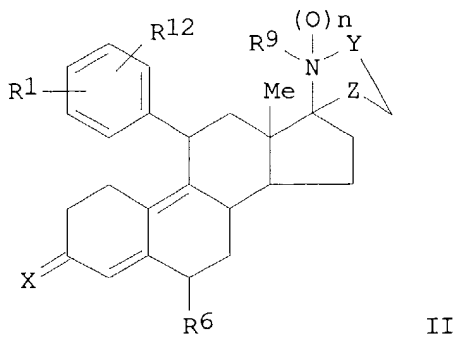
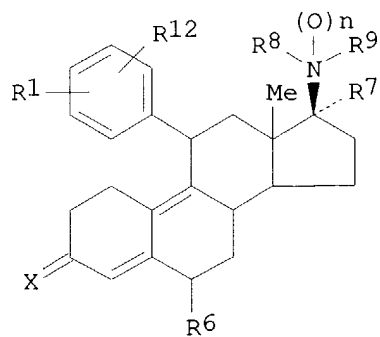
THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/611,785

applicant

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1999:784119 CAPLUS
 DOCUMENT NUMBER: 132:23141
 TITLE: Preparation of 17 β -amino- and
 17 β -hydroxylamino-11 β -arylsteroids with
 potent antiprogestational activity
 INVENTOR(S): Cook, C. Edgar; Kepler, John A.; Bartley, Gary S.;
 Shetty, Rupa S.
 PATENT ASSIGNEE(S): Research Triangle Institute, USA
 SOURCE: PCT Int. Appl., 75 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9962928	A1	19991209	WO 1999-US10480	19990528
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6262042	B1	20010717	US 1998-86560	19980529
CA 2333669	AA	19991209	CA 1999-2333669	19990528
AU 9950761	A1	19991220	AU 1999-40761	19990528
AU 753382	B2	20021017		
BR 9910794	A	20010213	BR 1999-10794	19990528
EP 1082337	A1	20010314	EP 1999-924207	19990528
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002531381	T2	20020924	JP 2000-552138	19990528
NZ 507985	A	20031128	NZ 1999-507985	19990528
NO 2000005989	A	20001127	NO 2000-5989	20001127
US 2002065257	A1	20020530	US 2001-895395	20010702
US 6620801	B2	20030916		
US 2004023936	A1	20040205	US 2003-611785	20030702
PRIORITY APPLN. INFO.:			US 1998-86560 A	19980529
			WO 1999-US10480 W	19990528
			US 2001-895395 A1	20010702
OTHER SOURCE(S):	MARPAT 132:23141			
GI				



AB 11 β -Phenylestradienes I [R1 = R2R3N(O)^m, nitrogen containing heterocyclyl; R2, R3 = H, alkyl, cycloalkyl alkenyl; R6 = H, alkyl, halogen; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R8, R9 = H, OH, alkyl, alkenyl, alkynyl, acyl, alkyloxy; R13 = H, halogen; R1R12 = fused nitrogen containing heterocyclic ring; X = H₂, OH, silyloxy, acyloxy, etc.; m, n = 0, 1] and II [R1 = R2R3N(O)^m, nitrogen containing heterocyclyl; R2, R3 = H, alkyl, cycloalkyl alkenyl; R6 = H, alkyl, halogen; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R9 = H, OH, alkyl, alkenyl, alkynyl, acyl, alkyloxy; R13 = H, halogen; R1R12 = fused nitrogen containing heterocyclic ring; X = H₂, OH, silyloxy, acyloxy, etc.; Y = CR13R14; Z = CH₂, C:CH₂; R13, R14 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R13R14 = O; m, n = 0, 1] were prepared and exhibited potent antiprogestational activity. Thus, oxime III (R = 4-dimethylaminophenyl) was prepared starting from sterol IV (R = 4-dimethylaminophenyl) in two steps. The prepared compds. were tested for progesterone receptor binding activity, progestational activity, and antiprogestational activity.

IT **251987-44-7P 251987-54-9P**

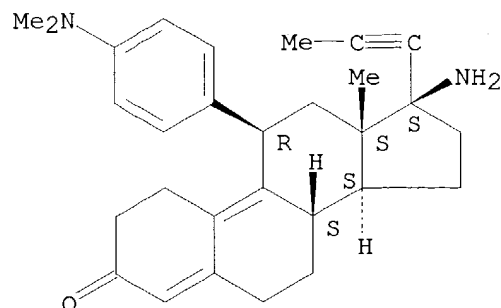
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of 17 β -amino- and 17 β -hydroxylamino-11 β -phenylestradienes with potent antiprogestational activity)

RN 251987-44-7 CAPLUS

CN Estra-4,9-dien-3-one, 17-amino-11-[4-(dimethylamino)phenyl]-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

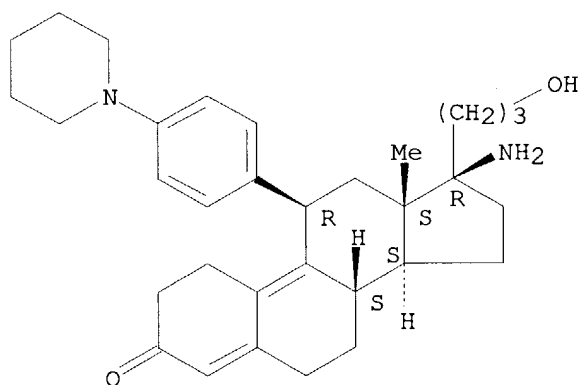
Absolute stereochemistry.



RN 251987-54-9 CAPLUS

CN Estra-4,9-dien-3-one, 17-amino-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 251987-35-6P 251987-40-3P 251987-48-1P
 251987-52-7P 251987-58-3P 251987-62-9P
 251987-65-2P 251988-38-2P 251988-39-3P
 251988-40-6P 251988-41-7P 251988-42-8P
 251988-43-9P 251988-45-1P 251988-46-2P
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 251988-54-2P 251988-55-3P

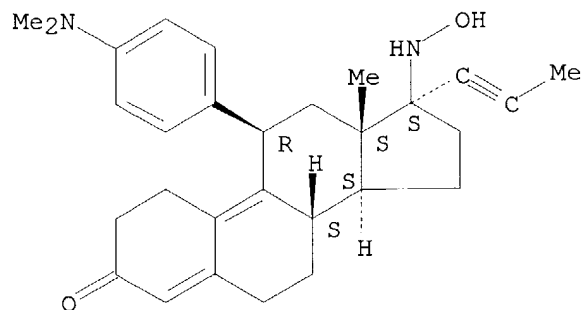
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 17 β -amino- and 17 β -hydroxylamino-11 β -phenylestradienes with potent antiprogestational activity)

RN 251987-35-6 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-(hydroxyamino)-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

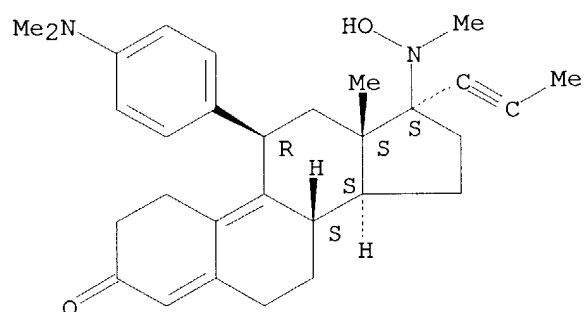
10/611,785



RN 251987-40-3 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-(hydroxymethylamino)-17-(1-propynyl)-, (11β,17β)- (9CI) (CA INDEX NAME)

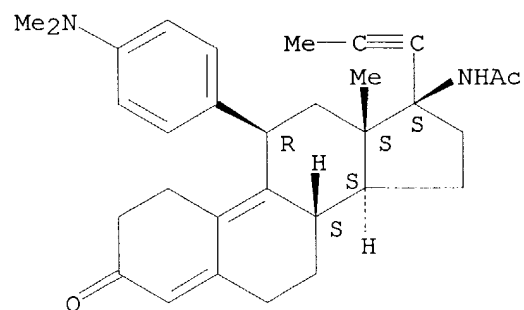
Absolute stereochemistry.



RN 251987-48-1 CAPLUS

CN Acetamide, N-[(11β,17β)-11-[4-(dimethylamino)phenyl]-3-oxo-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

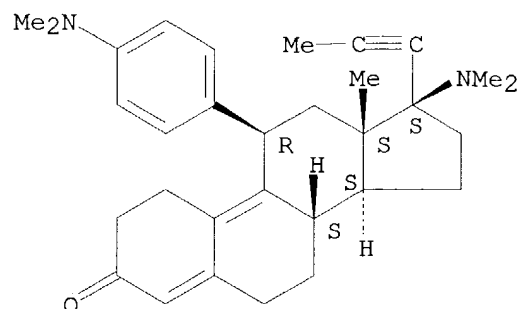


RN 251987-52-7 CAPLUS

CN Estra-4,9-dien-3-one, 17-(dimethylamino)-11-[4-(dimethylamino)phenyl]-17-(1-propynyl)-, (11β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

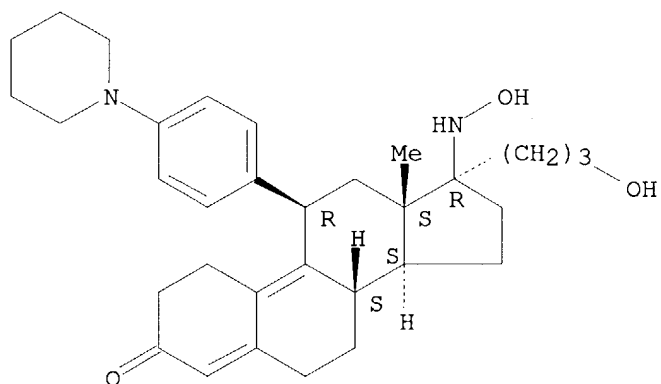
10/611,785



RN 251987-58-3 CAPLUS

CN Estr-4,9-dien-3-one, 17-(hydroxyamino)-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, (11 β ,17 β)-(9CI) (CA INDEX NAME)

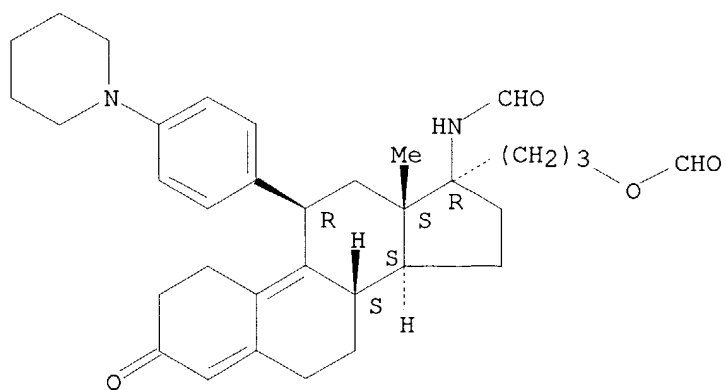
Absolute stereochemistry.



RN 251987-62-9 CAPLUS

CN Formamide, N-[(11 β ,17 β)-17-[3-(formyloxy)propyl]-3-oxo-11-[4-(1-piperidinyl)phenyl]estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

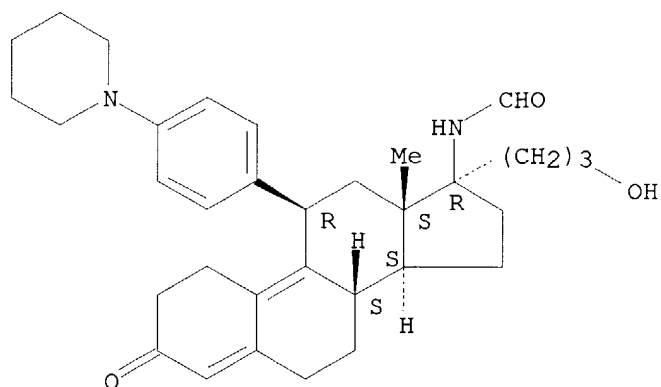


RN 251987-65-2 CAPLUS

10/611,785

CN Formamide, N-[(11 β ,17 β)-17-(3-hydroxypropyl)-3-oxo-11-[4-(1-piperidinyl)phenyl]estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

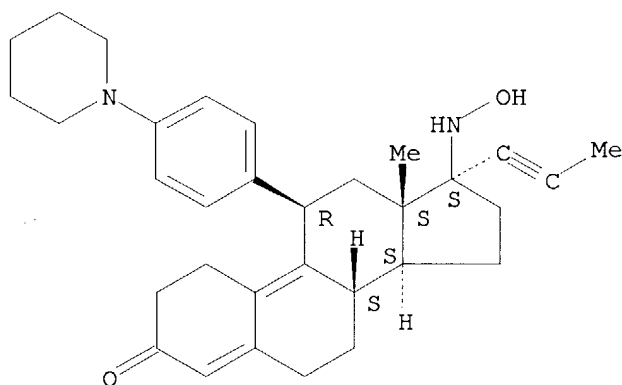
Absolute stereochemistry.



RN 251988-38-2 CAPLUS

CN Estradiol, 17-(hydroxyamino)-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

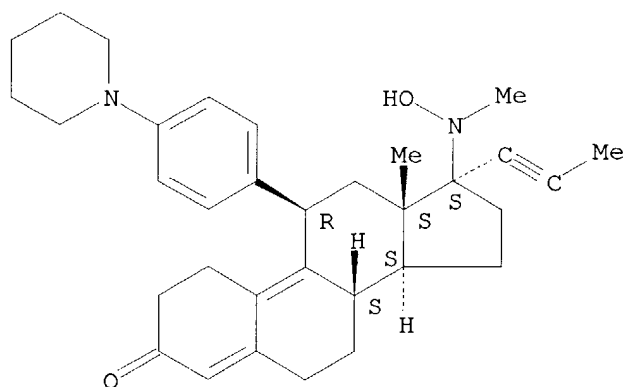
Absolute stereochemistry.



RN 251988-39-3 CAPLUS

CN Estradiol, 17-(hydroxymethylamino)-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

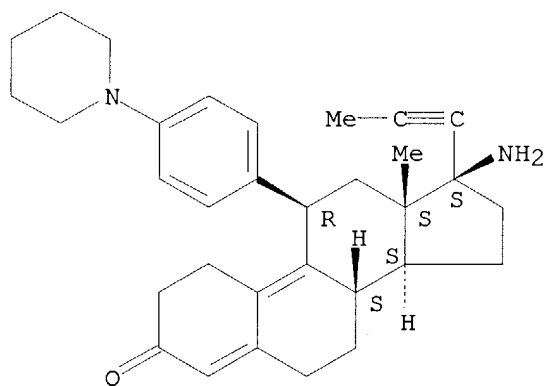
Absolute stereochemistry.



RN 251988-40-6 CAPLUS

CN Estradiol, 17-amino-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

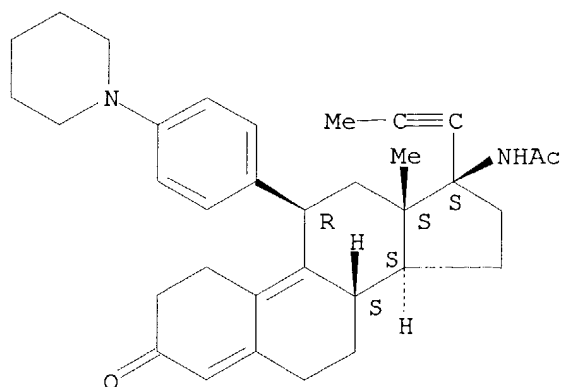
Absolute stereochemistry.



RN 251988-41-7 CAPLUS

CN Estradiol, N-[11 β ,17 β]-3-oxo-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

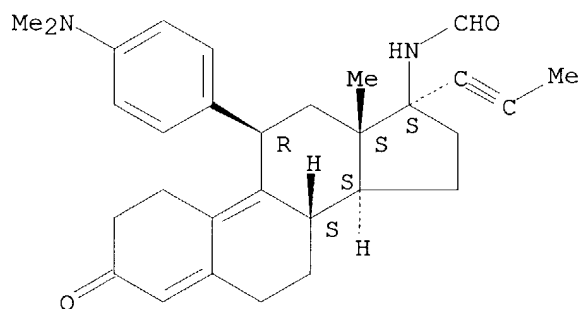
Absolute stereochemistry.



RN 251988-42-8 CAPLUS

CN Formamide, N-[(11β,17β)-11-[4-(dimethylamino)phenyl]-3-oxo-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

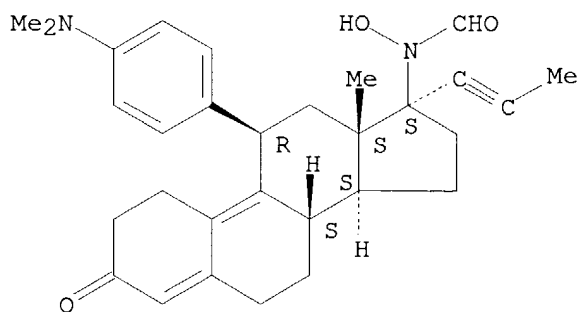
Absolute stereochemistry.



RN 251988-43-9 CAPLUS

CN Formamide, N-[(11β,17β)-11-[4-(dimethylamino)phenyl]-3-oxo-17-(1-propynyl)estra-4,9-dien-17-yl]-N-hydroxy- (9CI) (CA INDEX NAME)

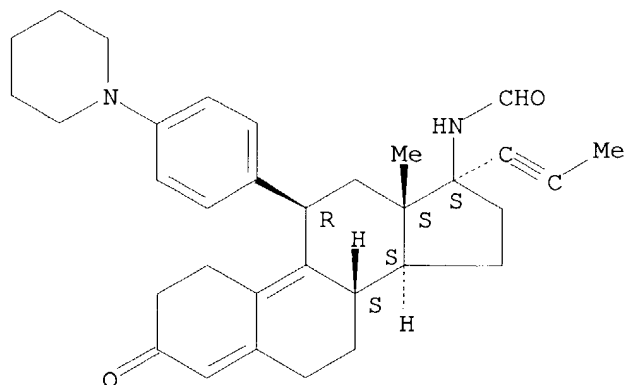
Absolute stereochemistry.



RN 251988-45-1 CAPLUS

CN Formamide, N-[(11β,17β)-3-oxo-11-[4-(1-piperidiny)phenyl]-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

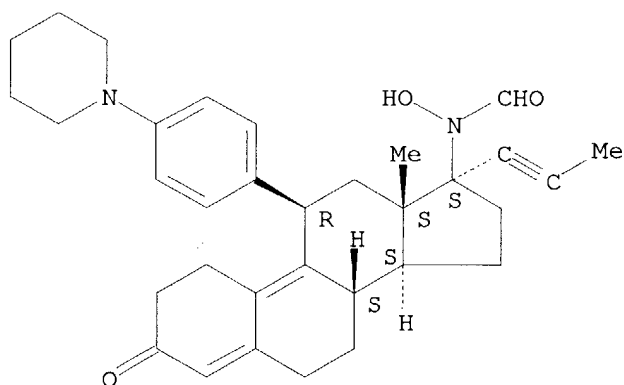
Absolute stereochemistry.



RN 251988-46-2 CAPLUS

CN Formamide, N-hydroxy-N-[(11 β ,17 β)-3-oxo-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

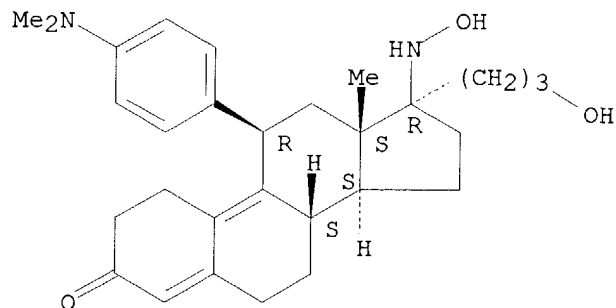
Absolute stereochemistry.



RN 251988-47-3 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-(hydroxyamino)-17-(3-hydroxypropyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

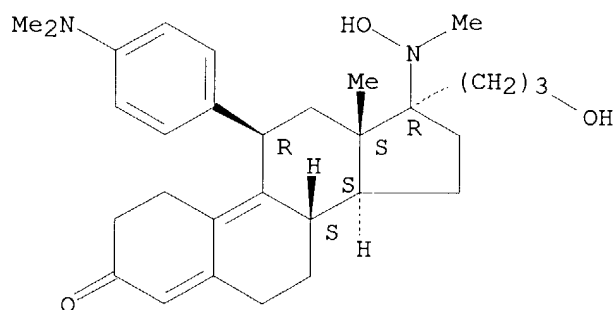
Absolute stereochemistry.



RN 251988-48-4 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-(hydroxymethylamino)-17-(3-hydroxypropyl)-, (11β,17β)- (9CI) (CA INDEX NAME)

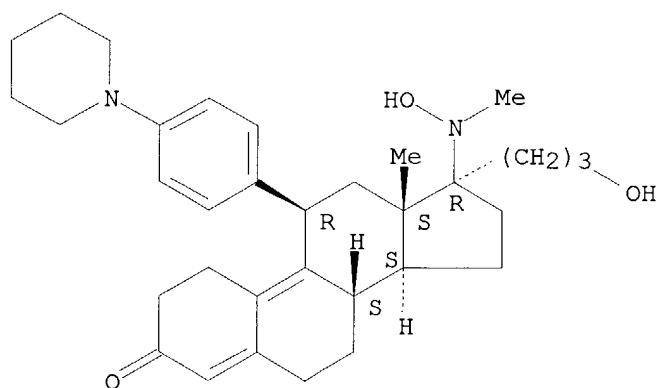
Absolute stereochemistry.



RN 251988-49-5 CAPLUS

CN Estra-4,9-dien-3-one, 17-(hydroxymethylamino)-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, (11β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

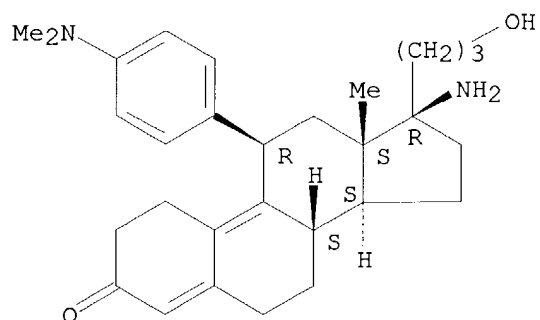


RN 251988-50-8 CAPLUS

CN Estra-4,9-dien-3-one, 17-amino-11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-, (11β,17β)- (9CI) (CA INDEX NAME)

10/611,785

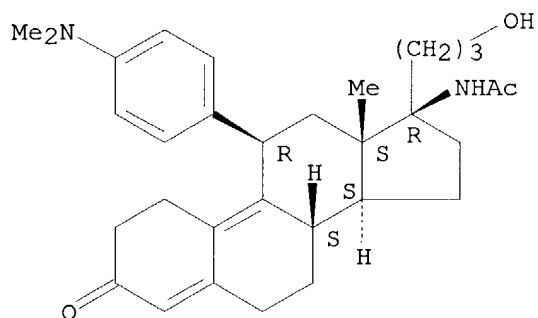
Absolute stereochemistry.



RN 251988-52-0 CAPLUS

CN Acetamide, N-[(11β,17β)-11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-3-oxoestra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

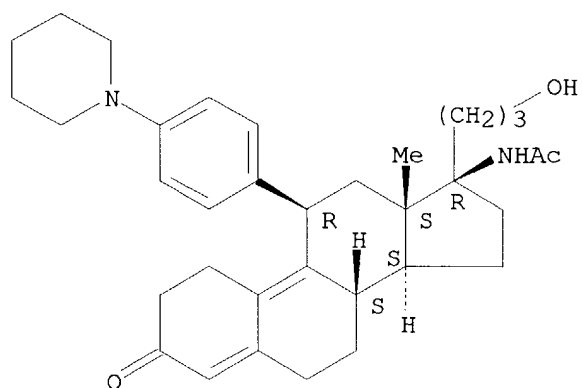
Absolute stereochemistry.



RN 251988-53-1 CAPLUS

CN Acetamide, N-[(11β,17β)-17-(3-hydroxypropyl)-3-oxo-11-[4-(1-piperidinyl)phenyl]estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

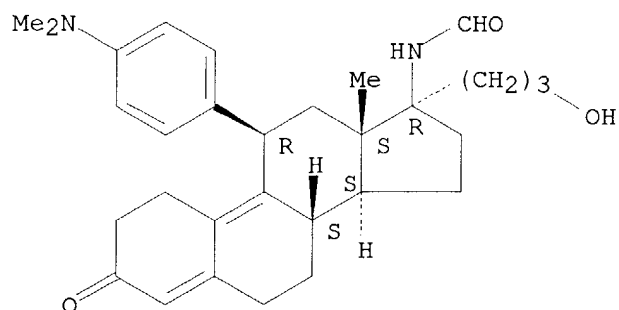


RN 251988-54-2 CAPLUS

10/611,785

CN Formamide, N-[(11 β ,17 β)-11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-3-oxoestra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

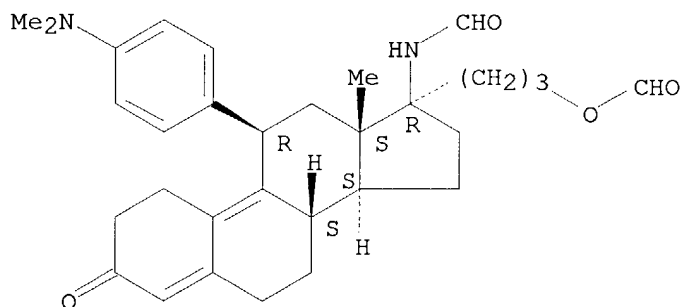
Absolute stereochemistry.



RN 251988-55-3 CAPLUS

CN Formamide, N-[(11 β ,17 β)-11-[4-(dimethylamino)phenyl]-17-[3-(formyloxy)propyl]-3-oxoestra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



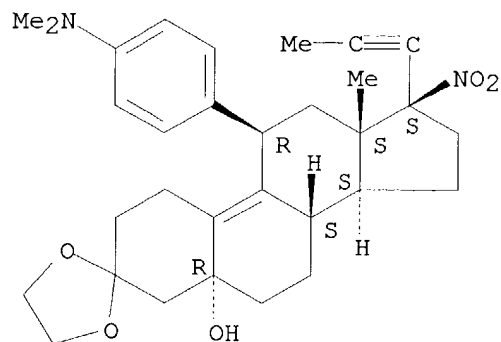
IT **244305-29-1 251988-37-1**

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 17 β -amino- and 17 β -hydroxylamino-11 β -phenylestradienes with potent antiprogestational activity)

RN 244305-29-1 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

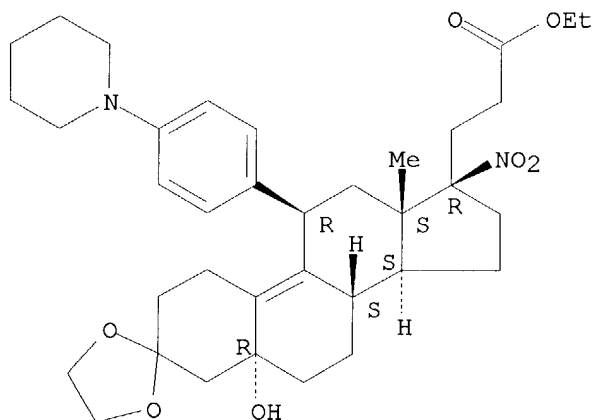
Absolute stereochemistry.



RN 251988-37-1 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, ethyl ester, (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 251987-79-8P 251987-83-4P 251987-87-8P

251988-11-1P 251988-14-4P 251988-17-7P

251988-20-2P 251988-22-4P 251988-24-6P

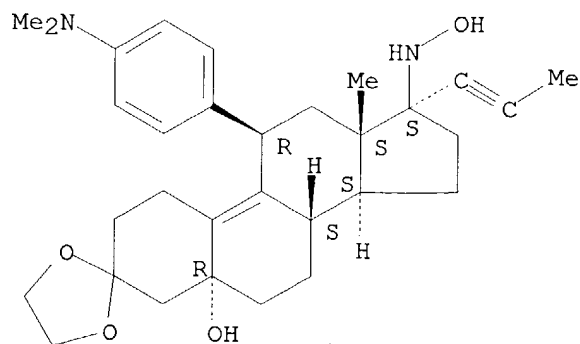
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 17 β -amino- and 17 β -hydroxylamino-11 β -phenylestradienes with potent antiprogestational activity)

RN 251987-79-8 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-(hydroxyamino)-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

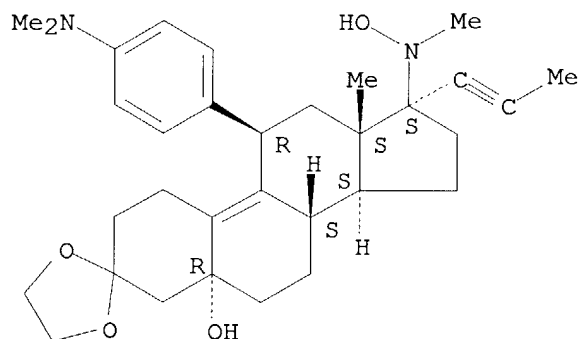
Absolute stereochemistry.



RN 251987-83-4 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-(hydroxymethylamino)-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

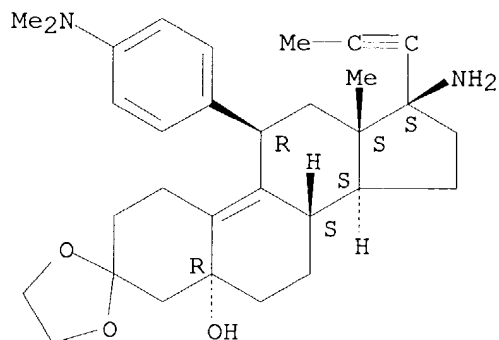
Absolute stereochemistry.



RN 251987-87-8 CAPLUS

CN Estr-9-en-3-one, 17-amino-11-[4-(dimethylamino)phenyl]-5-hydroxy-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

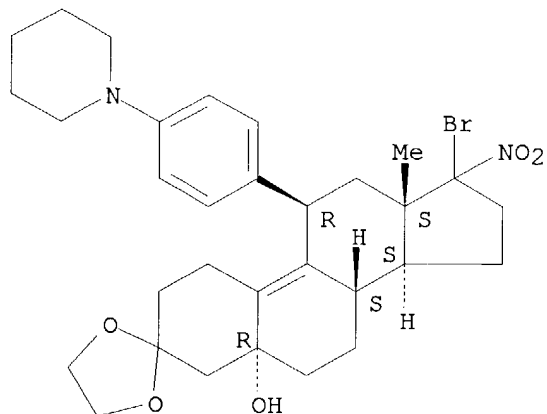


RN 251988-11-1 CAPLUS

10/611,785

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-
, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX
NAME)

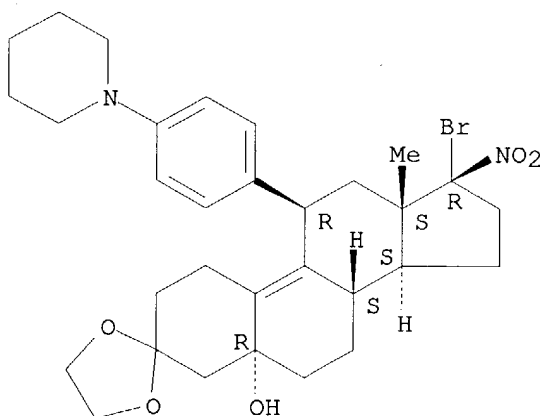
Absolute stereochemistry.



RN 251988-14-4 CAPLUS

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-
, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 α)- (9CI) (CA
INDEX NAME)

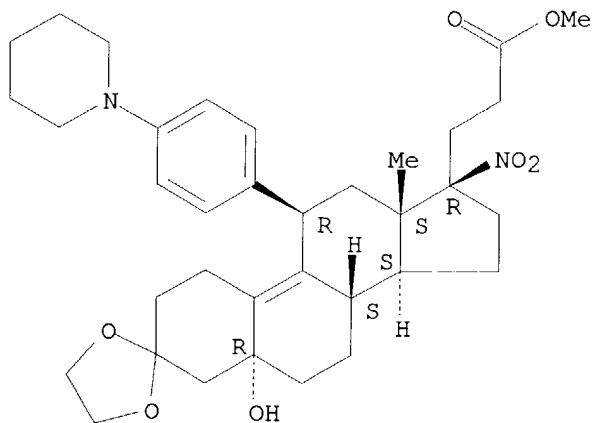
Absolute stereochemistry.



RN 251988-17-7 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-
hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, methyl ester,
(5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

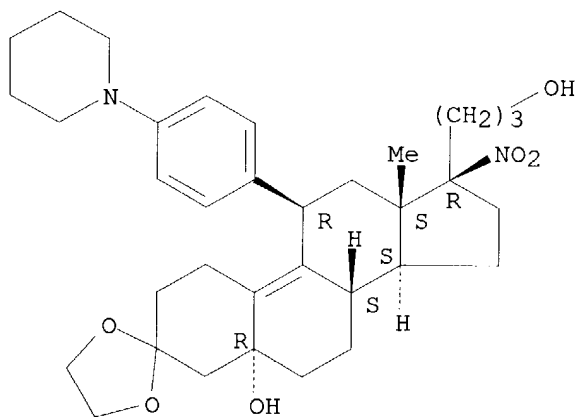
Absolute stereochemistry.



RN 251988-20-2 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

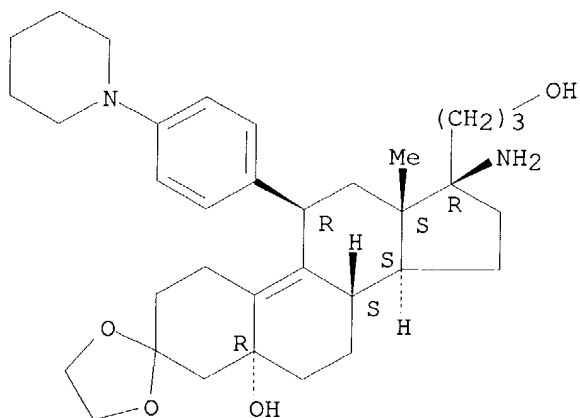
Absolute stereochemistry.



RN 251988-22-4 CAPLUS

CN Estr-9-en-3-one, 17-amino-5-hydroxy-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

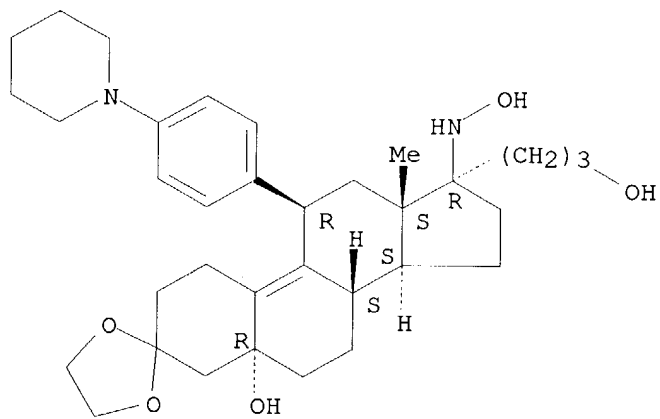
Absolute stereochemistry.



RN 251988-24-6 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(hydroxyamino)-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:633297 CAPLUS

DOCUMENT NUMBER: 131:243468

TITLE: Preparation of 17 β -nitro-11 β -arylsteroids and their derivatives having agonist or antagonist hormonal properties

INVENTOR(S): Cook, C. Edgar; Kepler, John A.; Shetty, Rupa S.; Bartley, Gary S.; Lee, David Yue-Wei

PATENT ASSIGNEE(S): Research Triangle Institute, USA

SOURCE: U.S., 24 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

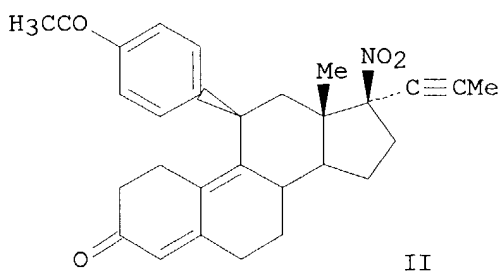
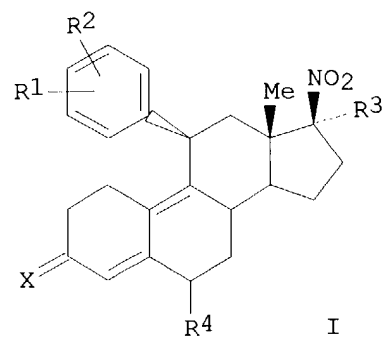
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5962444	A	19991005	US 1998-86674	19980529
US 6015805	A	20000118	US 1999-317945	19990525
CA 2333668	AA	19991209	CA 1999-2333668	19990528
WO 9962929	A1	19991209	WO 1999-US10481	19990528
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BE, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9940762	A1	19991220	AU 1999-40762	19990528
AU 753355	B2	20021017		
EP 1082338	A1	20010314	EP 1999-924208	19990528
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002517405	T2	20020618	JP 2000-552139	19990528
US 6093707	A	20000725	US 1999-434473	19991105
PRIORITY APPLN. INFO.:			US 1998-86674	A3 19980529
			US 1999-317945	A3 19990525
			WO 1999-US10481	W 19990528

OTHER SOURCE(S): MARPAT 131:243468

GI



AB 17 β -Nitro-11 β -arylsteroids of formula I [R1 = (substituted) amino, halo, OH, alkoxy, alkylthio, acyl, etc.; R2 = H, halo; R3 = H, alkyl, alkenyl, alkynyl, aryl, etc.; R4 = H, alkyl, halo; X = O, (substituted) NOH] are prepared. The compds. exhibit potent antiprogestational activity and are useful in the treatment of fibroids, endometriosis, cervical ripening prior to delivery, hormone replacement therapy and in the control of fertility. Thus, 3,3-(1,2-ethanedioxy)estra-5(10),9(11)-dien-17-one was transformed into II in several steps. The affinity of II for human progesterone hormone receptor was IC₅₀ of 0.8 nM.

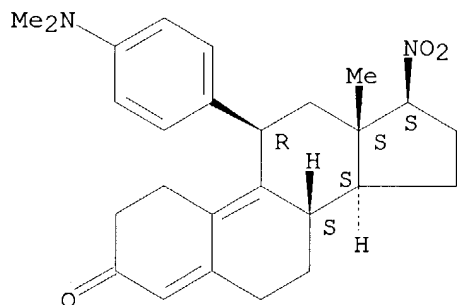
IT **244304-80-1P 244304-81-2P 244304-82-3P**
244304-83-4P 244304-84-5P 244304-85-6P
244304-86-7P 244304-89-0P 244304-90-3P
244304-91-4P 244305-03-1P 244305-17-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 17 β -nitro-11 β -arylsteroids and derivs. with
 progestational or antiprogestational activity)

RN 244304-80-1 CAPLUS

CN Estr-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-nitro-,
 (11 β ,17 β)- (9CI) (CA INDEX NAME)

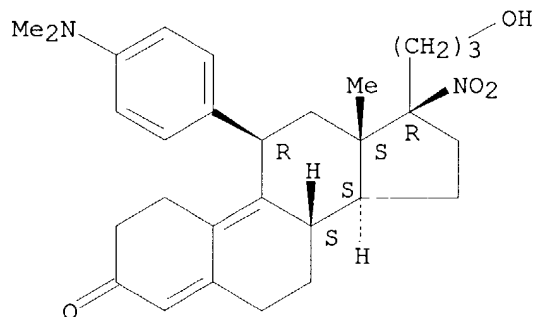
Absolute stereochemistry.



RN 244304-81-2 CAPLUS

CN Estr-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

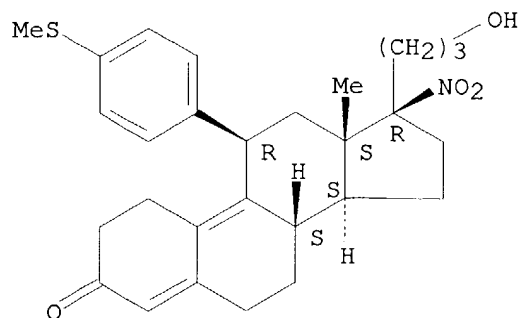


RN 244304-82-3 CAPLUS

10/611,785

CN Estr-4,9-dien-3-one, 17-(3-hydroxypropyl)-11-[4-(methylthio)phenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

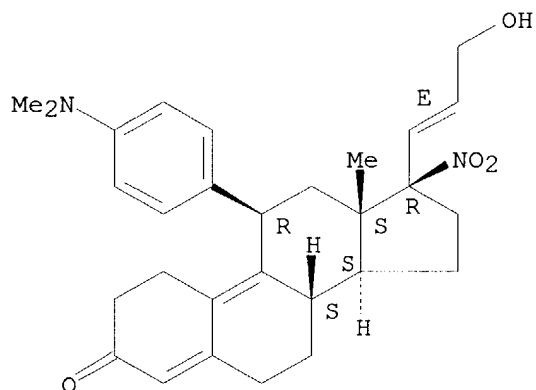


RN 244304-83-4 CAPLUS

CN Estr-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



RN 244304-84-5 CAPLUS

CN Estr-4,9-dien-3-one, 11-(4-acetylphenyl)-17-(3-hydroxypropyl)-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

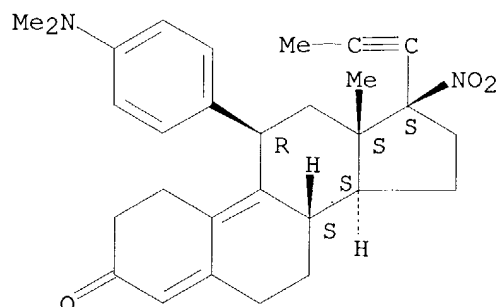
Absolute stereochemistry.

10/611,785

RN 244304-89-0 CAPLUS

CN Estr-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-nitro-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

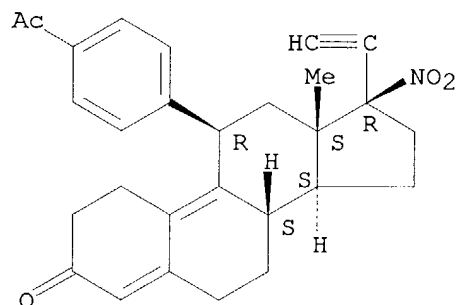
Absolute stereochemistry.



RN 244304-90-3 CAPLUS

CN 19-Norpregna-4,9-dien-20-yn-3-one, 11-(4-acetylphenyl)-17-nitro-, (11 β ,17 α)- (9CI) (CA INDEX NAME)

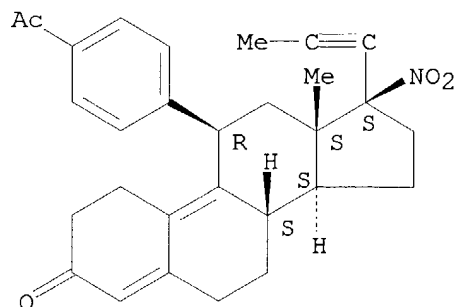
Absolute stereochemistry.



RN 244304-91-4 CAPLUS

CN Estr-4,9-dien-3-one, 11-(4-acetylphenyl)-17-nitro-17-(1-propynyl)-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



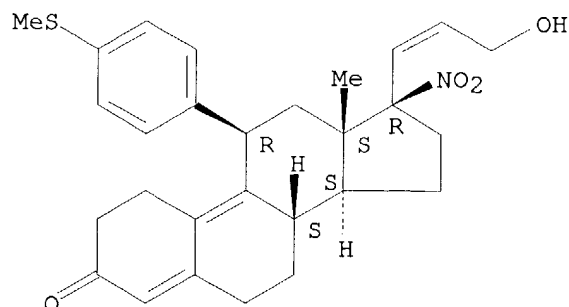
RN 244305-03-1 CAPLUS

10/611,785

CN Estr-4,9-dien-3-one, 17-(3-hydroxy-1-propenyl)-11-[4-(methylthio)phenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

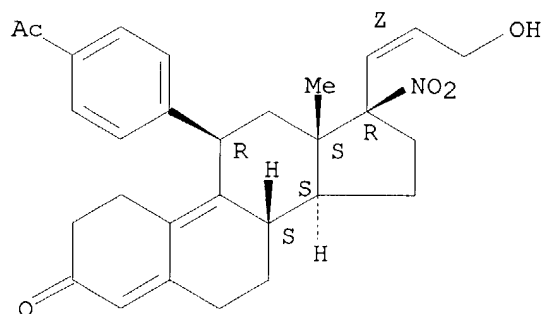


RN 244305-17-7 CAPLUS

CN Estr-4,9-dien-3-one, 11-(4-acetylphenyl)-17-[(1Z)-3-hydroxy-1-propenyl]-17-nitro-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT **244305-38-2**

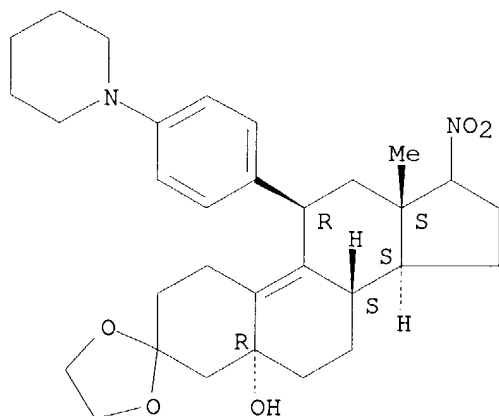
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 17 β -nitro-11 β -arylsteroids and derivs. with progestational or antiprogestational activity)

RN 244305-38-2 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 244304-96-9P 244304-97-0P 244304-98-1P
 244304-99-2P 244305-00-8P 244305-01-9P
 244305-02-0P 244305-04-2P 244305-06-4P
 244305-07-5P 244305-09-7P 244305-10-0P
 244305-11-1P 244305-12-2P 244305-13-3P
 244305-14-4P 244305-15-5P 244305-16-6P
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 244305-22-4P 244305-23-5P 244305-24-6P
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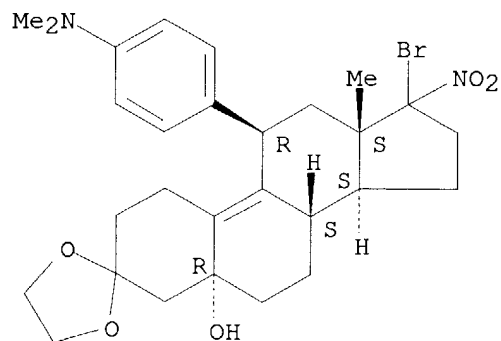
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 17 β -nitro-11 β -arylsteroids and derivs. with progestational or antiprogestational activity)

RN 244304-96-9 CAPLUS

CN Estr-9-en-3-one, 17-bromo-11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

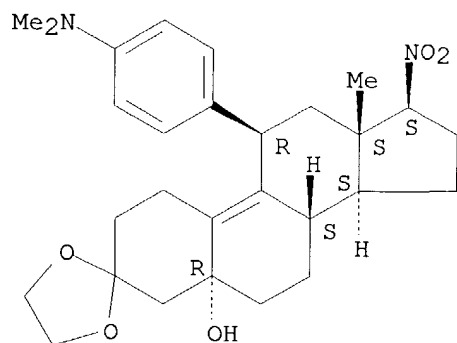


RN 244304-97-0 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

10/611,785

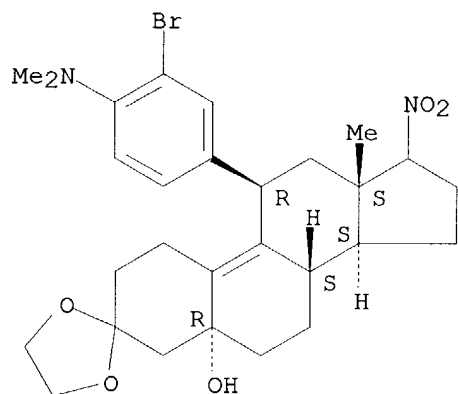
Absolute stereochemistry.



RN 244304-98-1 CAPLUS

CN Estr-9-en-3-one, 11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX NAME)

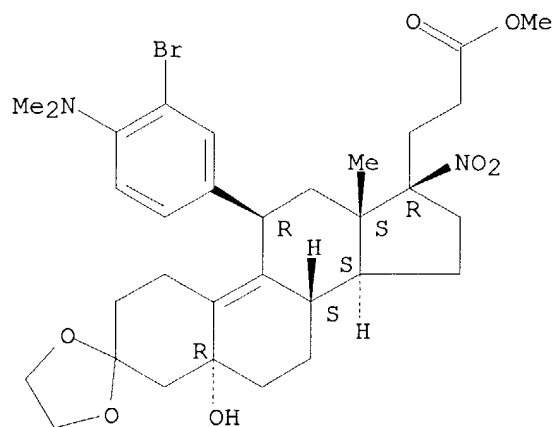
Absolute stereochemistry.



RN 244304-99-2 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 11-[3-bromo-4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

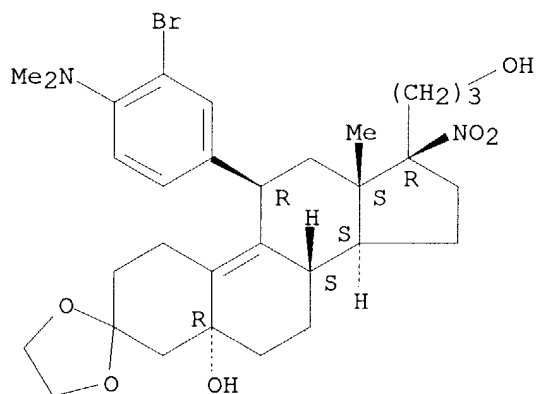
Absolute stereochemistry.



RN 244305-00-8 CAPLUS

CN Estr-9-en-3-one, 11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-(3-hydroxypropyl)-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

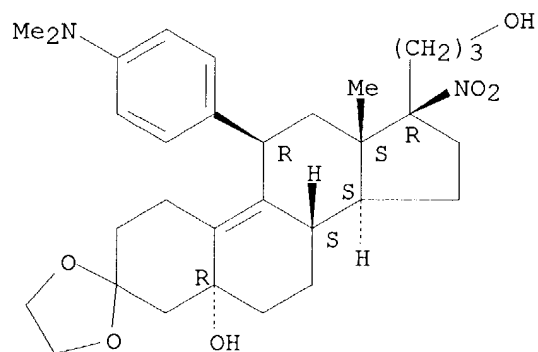
Absolute stereochemistry.



RN 244305-01-9 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-(3-hydroxypropyl)-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

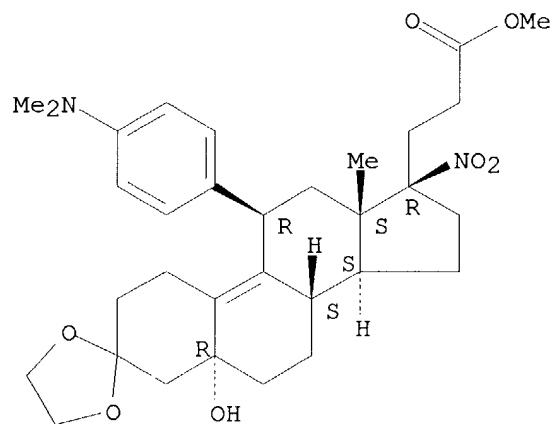
Absolute stereochemistry.



RN 244305-02-0 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 11-[4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

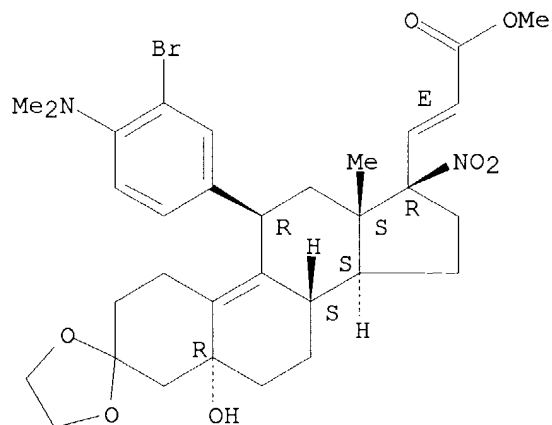


RN 244305-04-2 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, 11-[3-bromo-4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, (5 α ,11 β ,17 α ,20E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

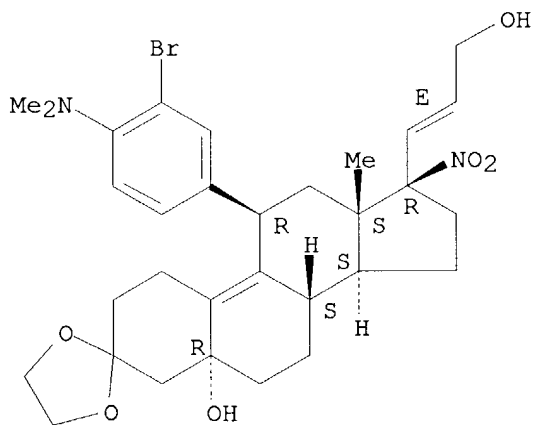


RN 244305-06-4 CAPLUS

CN Estr-9-en-3-one, 11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

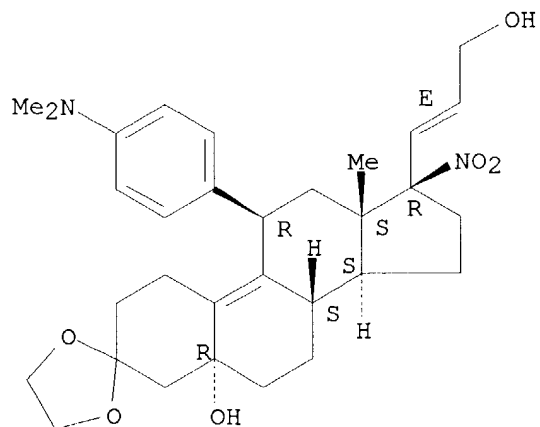


RN 244305-07-5 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

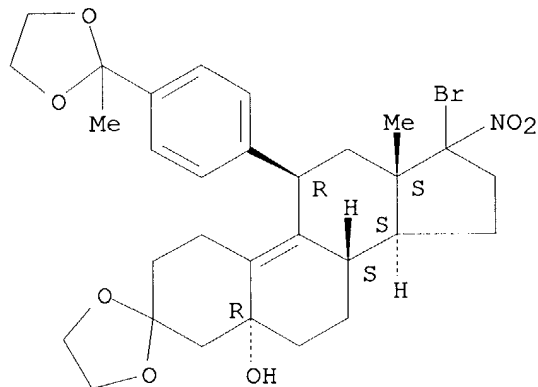
Double bond geometry as shown.



RN 244305-09-7 CAPLUS

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

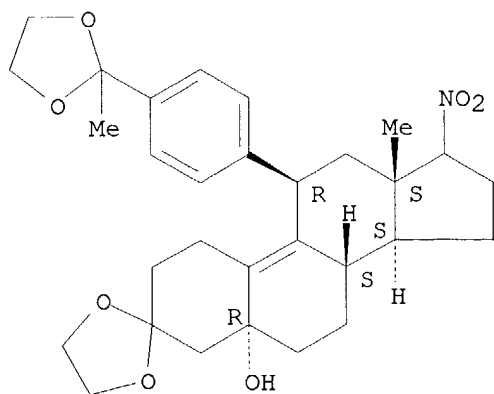


RN 244305-10-0 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

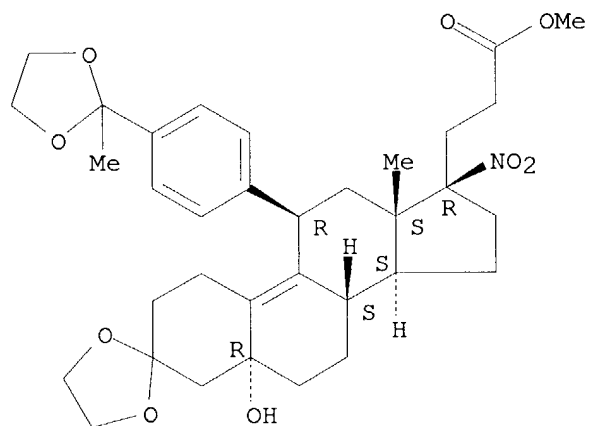
10/611,785



RN 244305-11-1 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, methyl ester, (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

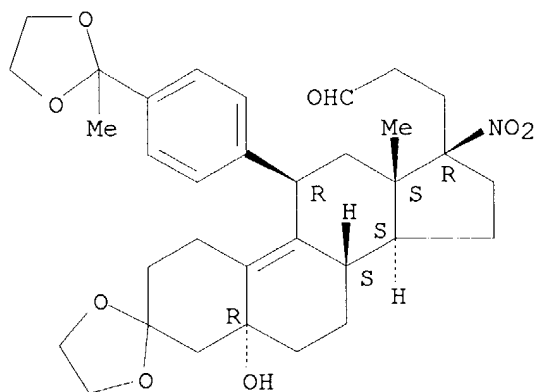
Absolute stereochemistry.



RN 244305-12-2 CAPLUS

CN 19-Norpregn-9-ene-21-carboxaldehyde, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

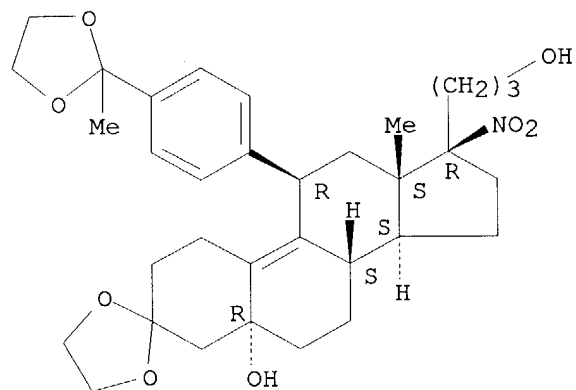
Absolute stereochemistry.



RN 244305-13-3 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

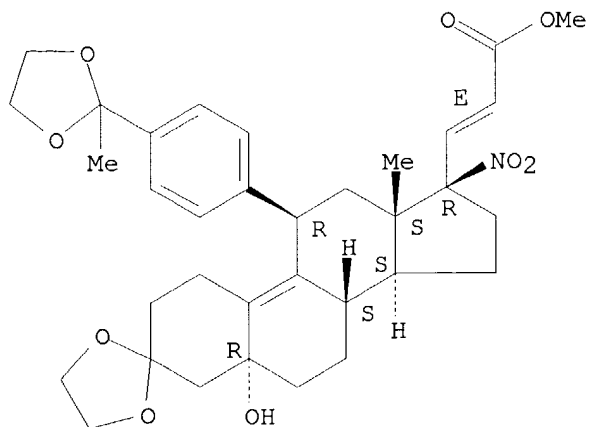


RN 244305-14-4 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, methyl ester, (5 α ,11 β ,17 α ,20E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

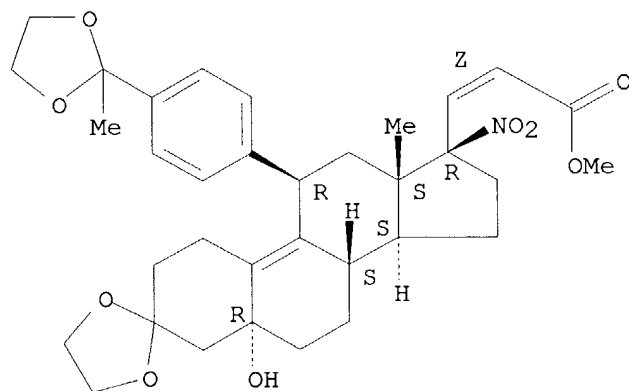


RN 244305-15-5 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, methyl ester, (5 α ,11 β ,17 α ,20Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

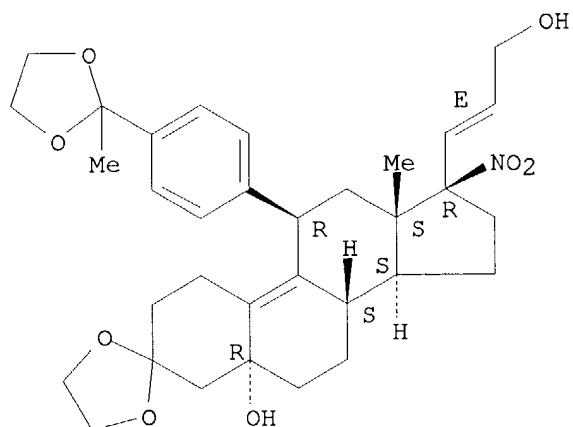


RN 244305-16-6 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-[(1E)-3-hydroxy-1-propenyl]-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

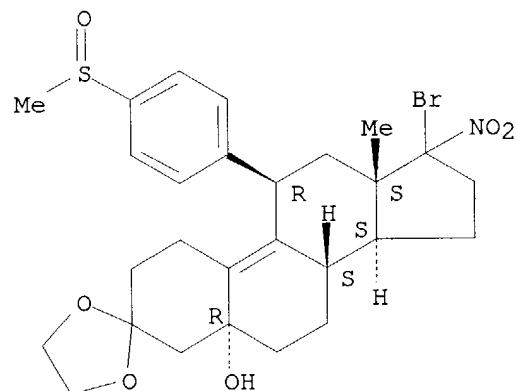
Double bond geometry as shown.



RN 244305-19-9 CAPLUS

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-11-[4-(methylsulfinyl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX NAME)

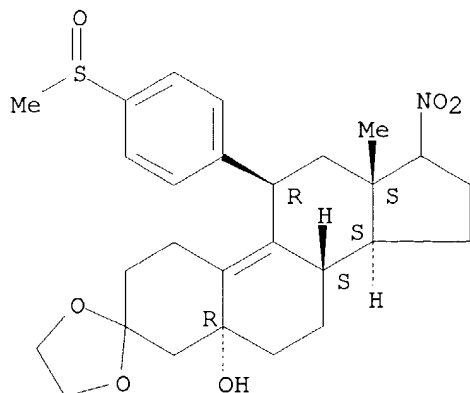
Absolute stereochemistry.



RN 244305-20-2 CAPLUS

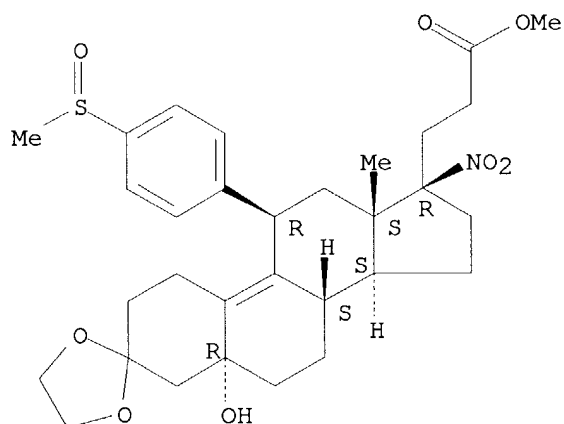
CN Estr-9-en-3-one, 5-hydroxy-11-[4-(methylsulfinyl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



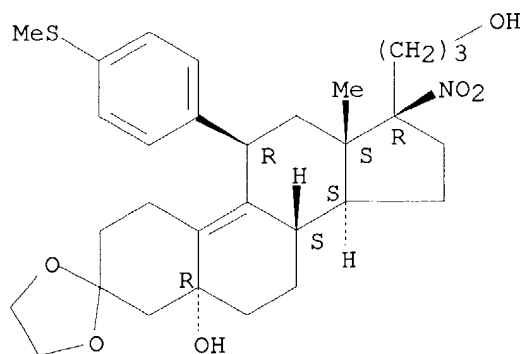
RN 244305-21-3 CAPLUS
 CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(methylsulfinyl)phenyl]-17-nitro-, methyl ester, (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 244305-22-4 CAPLUS
 CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-11-[4-(methylthio)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

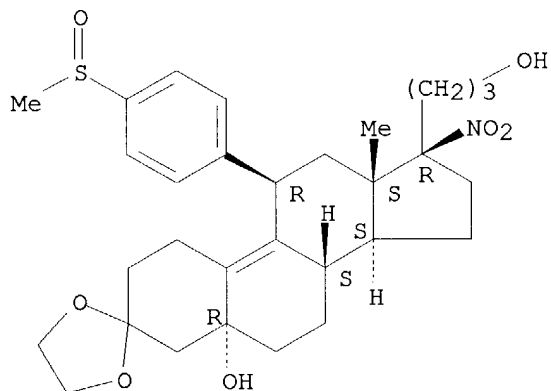
Absolute stereochemistry.



RN 244305-23-5 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-11-[4-(methylsulfinyl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

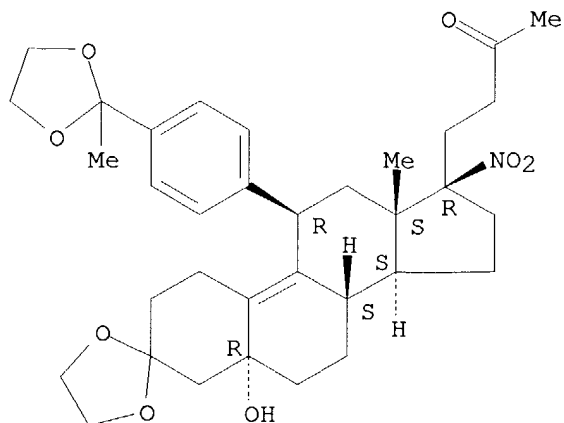
Absolute stereochemistry.



RN 244305-24-6 CAPLUS

CN 19,21-Dinorchol-9-ene-3,23-dione, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 3-(1,2-ethanediyl acetal), (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

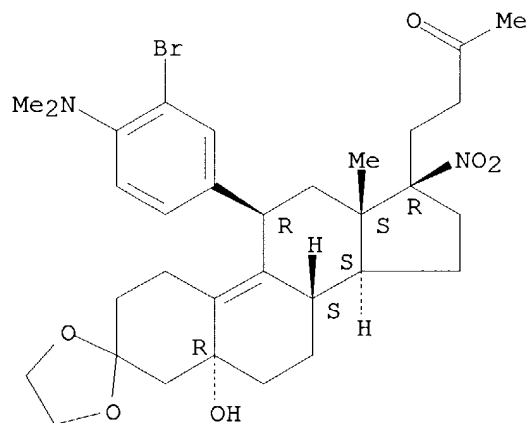
Absolute stereochemistry.



RN 244305-26-8 CAPLUS

CN 19,21-Dinorchol-9-ene-3,23-dione, 11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-, cyclic 3-(1,2-ethanediyl acetal), (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

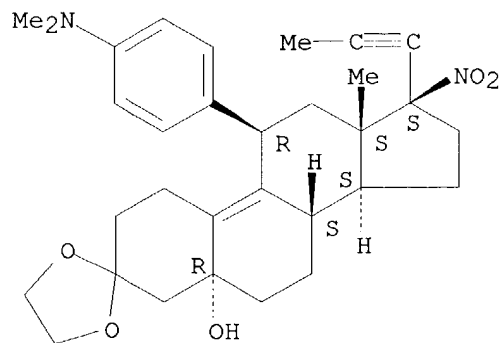
Absolute stereochemistry.



RN 244305-29-1 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

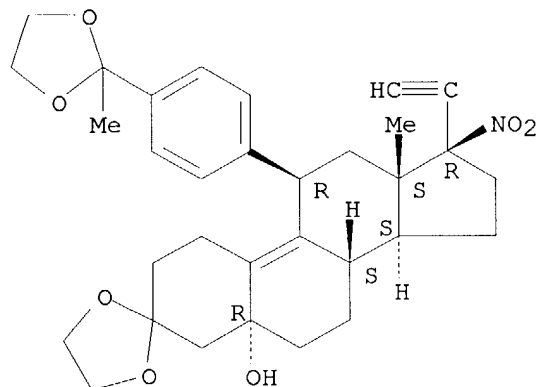
Absolute stereochemistry.



RN 244305-32-6 CAPLUS

CN 19-Norpregn-9-en-20-yn-3-one, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 α)- (9CI) (CA INDEX NAME)

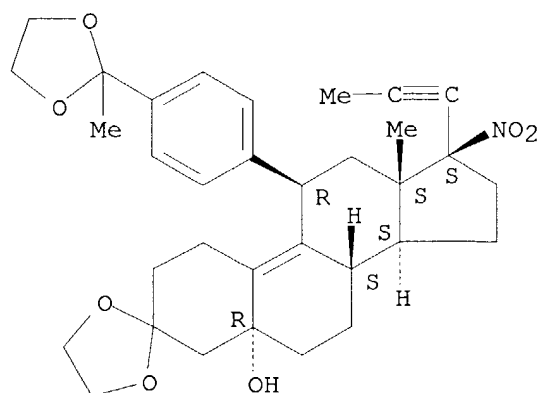
Absolute stereochemistry.



RN 244305-33-7 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

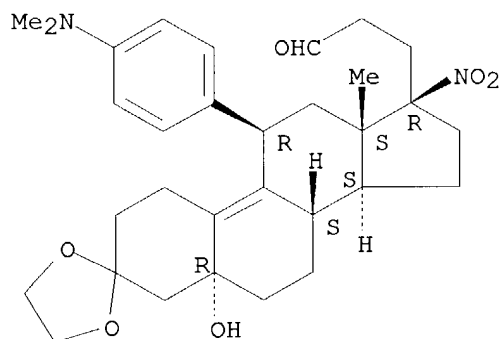
Absolute stereochemistry.



RN 244305-34-8 CAPLUS

CN 19-Norpregn-9-ene-21-carboxaldehyde, 11-[4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, (5 α ,11 β ,17 α)-(9CI) (CA INDEX NAME)

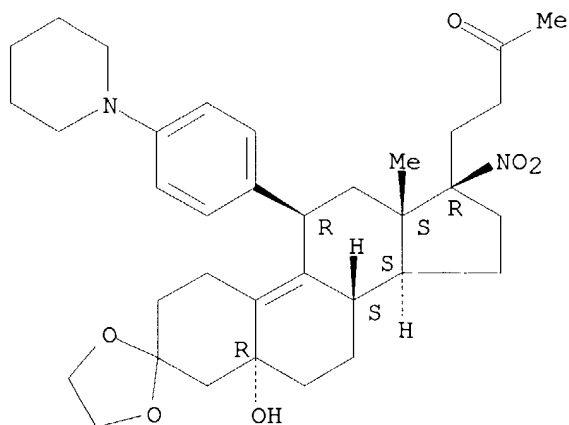
Absolute stereochemistry.



RN 244305-36-0 CAPLUS

CN 19,21-Dinorchol-9-ene-3,23-dione, 5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 3-(1,2-ethanediyl acetal), (5 α ,11 β ,17 α)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



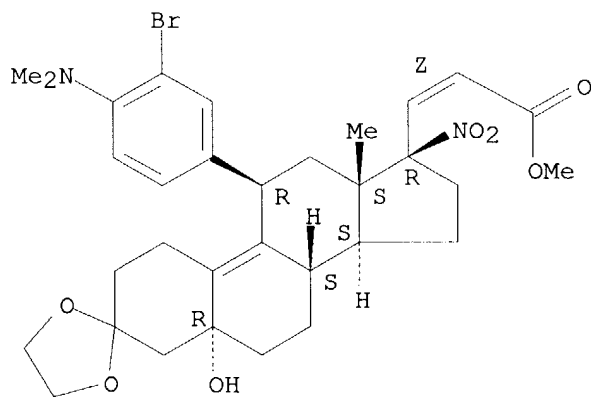
IT **244305-05-3P 244305-30-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 17 β -nitro-11 β -arylsteroids and derivs. with
progestational or antiprogestational activity)

RN 244305-05-3 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, 11-[3-bromo-4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, (5 α ,11 β ,17 α ,20Z)- (9CI) (CA INDEX NAME)

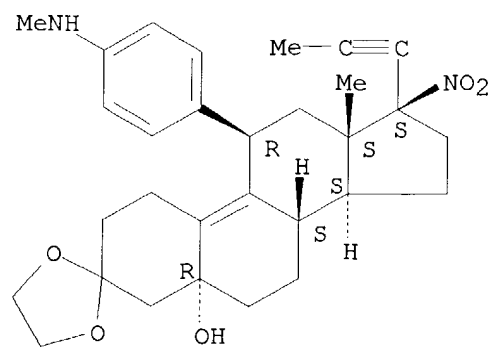
Absolute stereochemistry.
Double bond geometry as shown.



RN 244305-30-4 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-11-[4-(methylamino)phenyl]-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, (5 α ,11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

47

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RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT